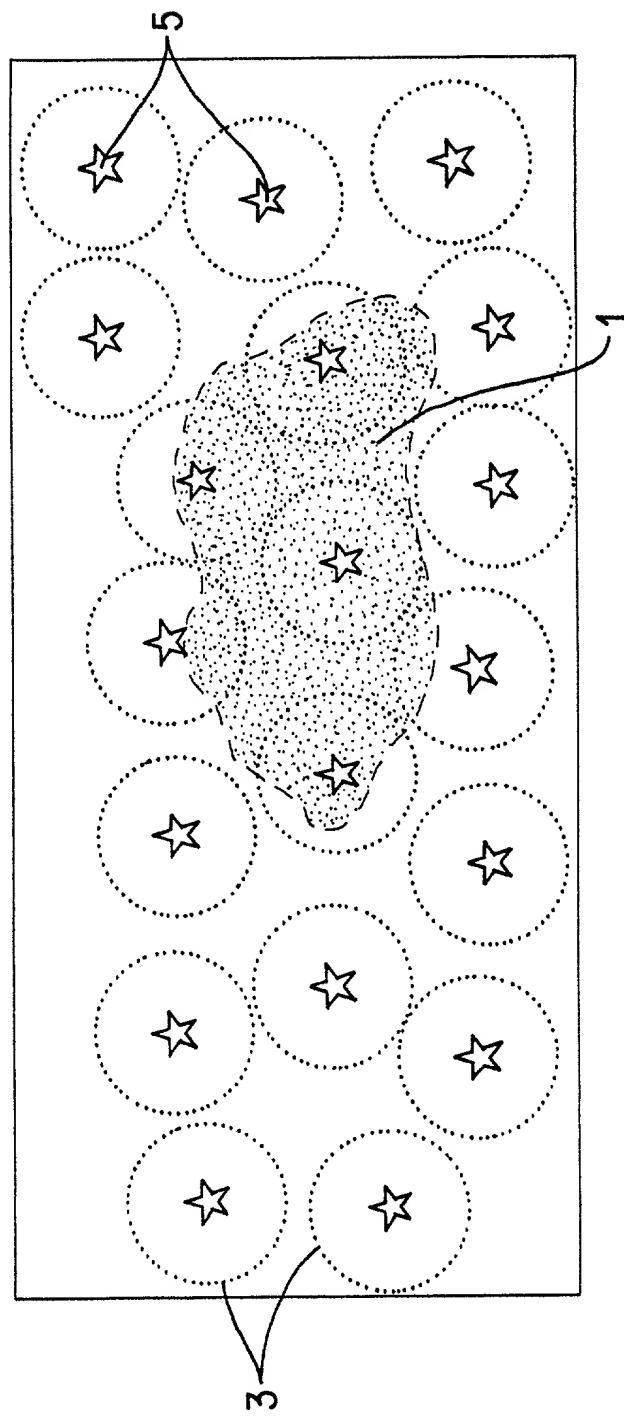


FIG. 1(a)

5#

FIG. 1(b)



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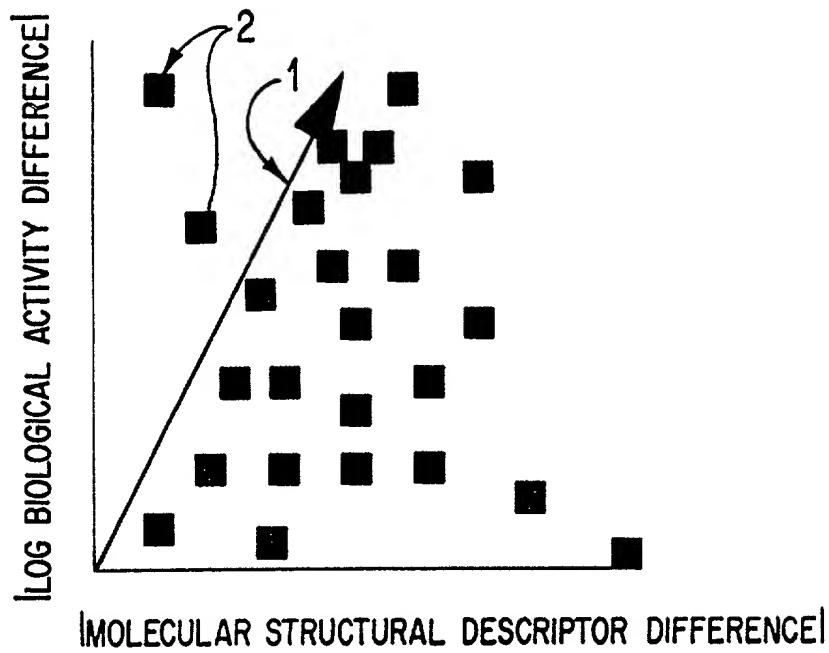


FIG. 2

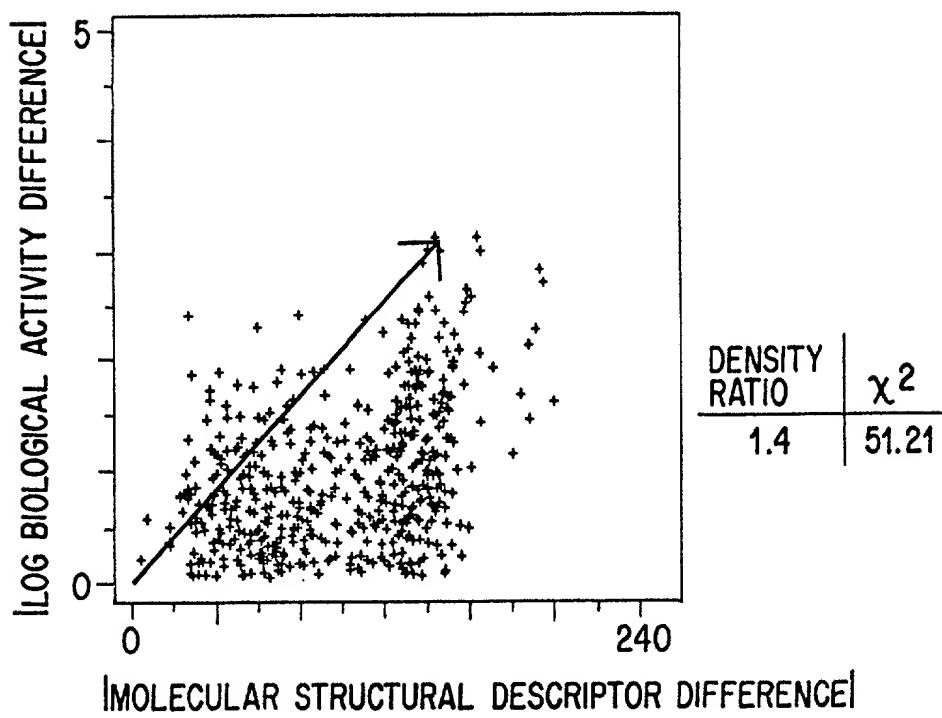


FIG. 3

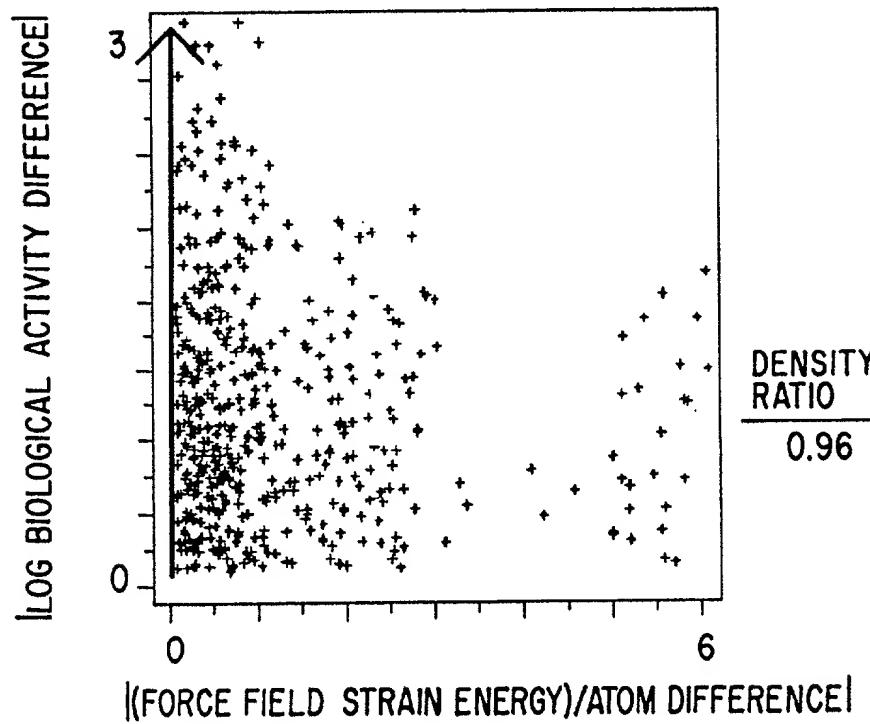
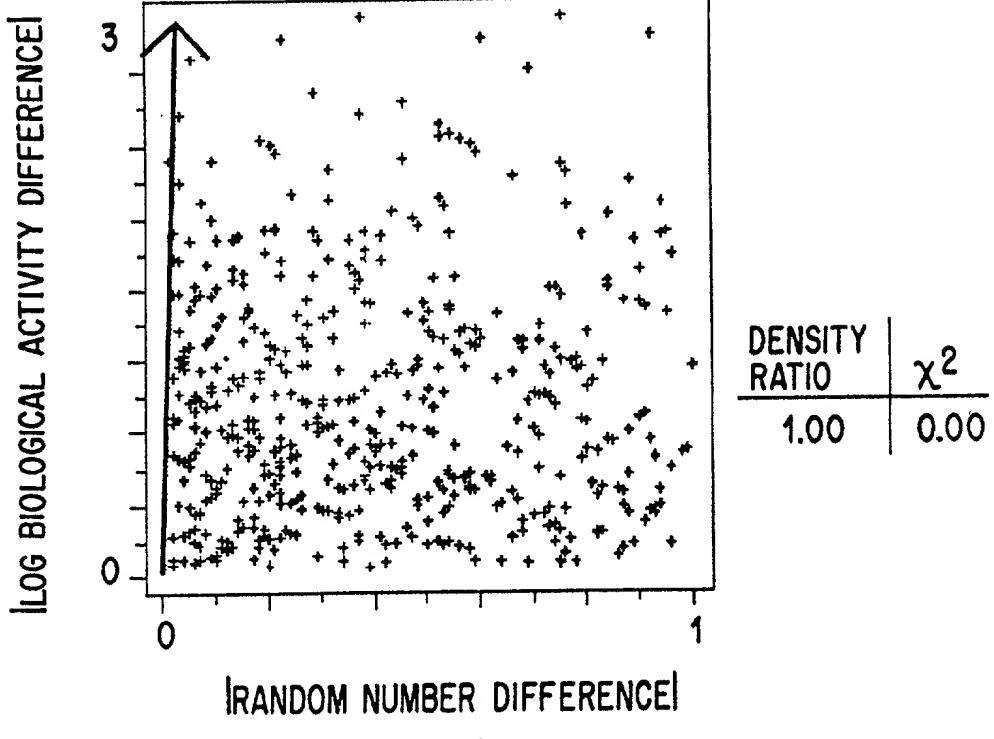


FIG. 5

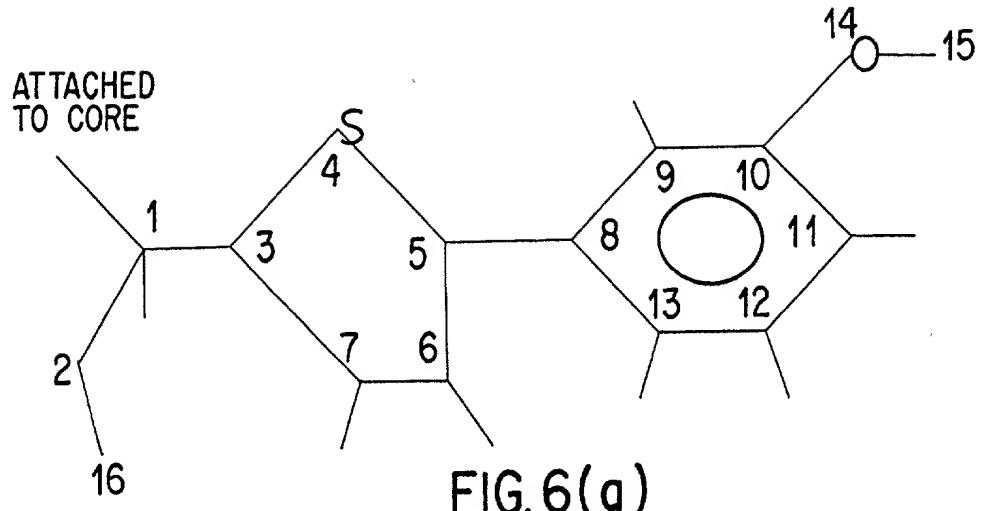


FIG. 6(a)

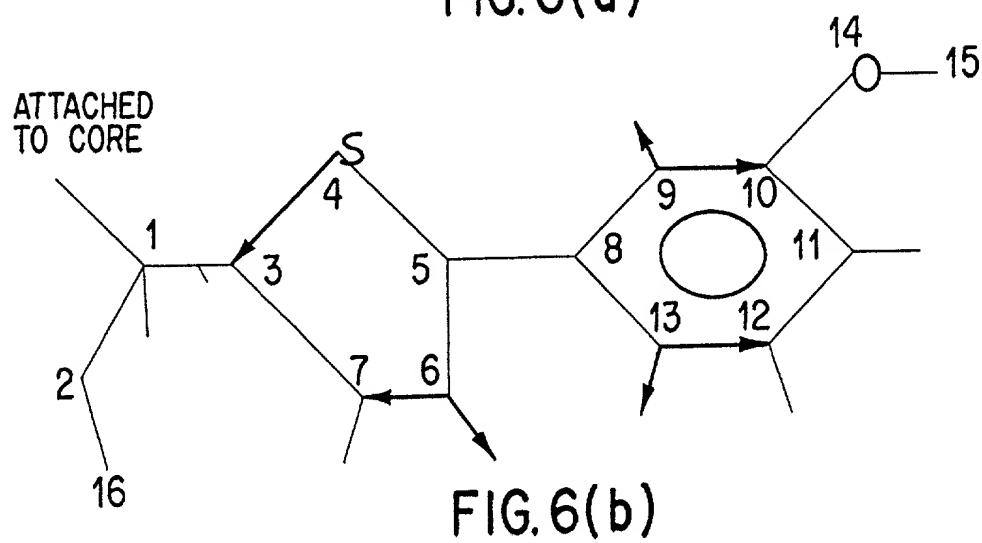


FIG. 6(b)

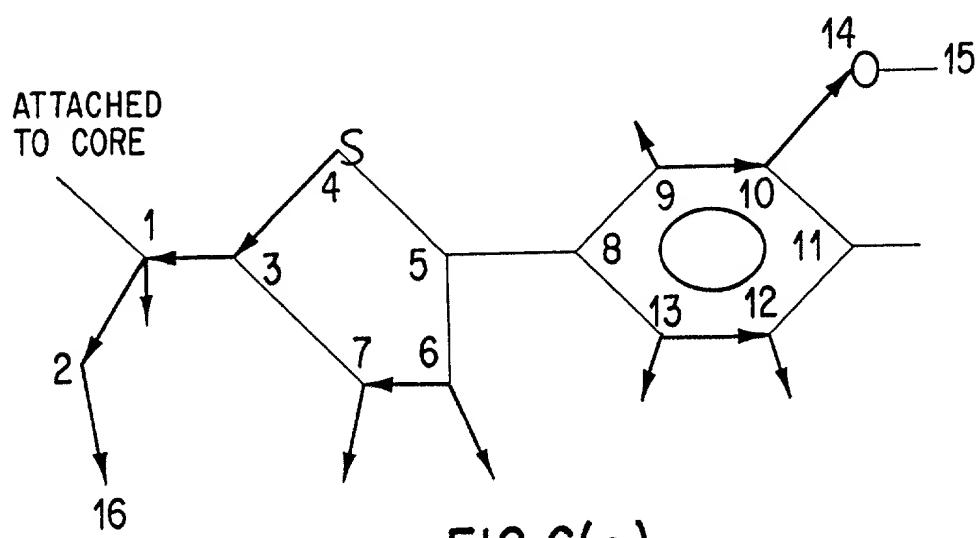


FIG. 6(c)

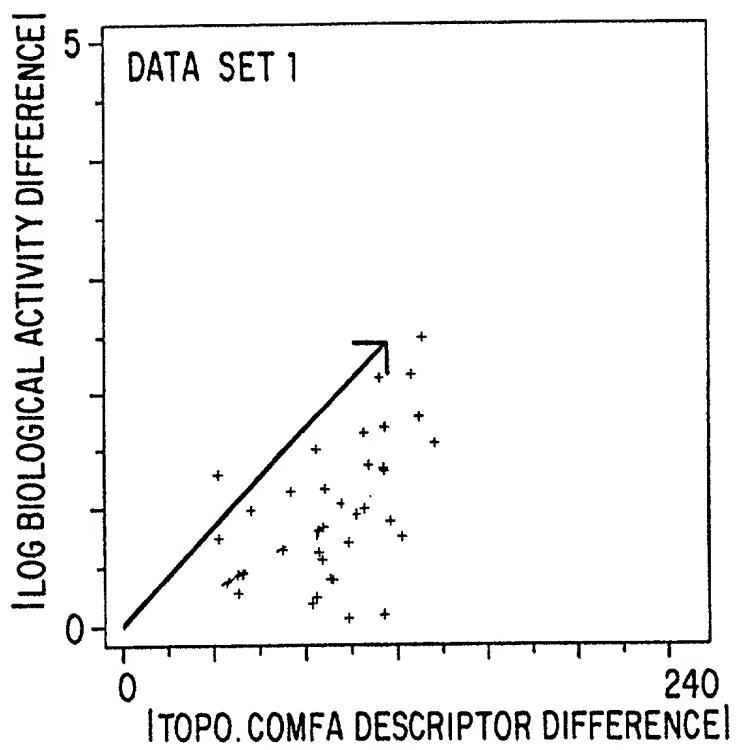


FIG.7(a)

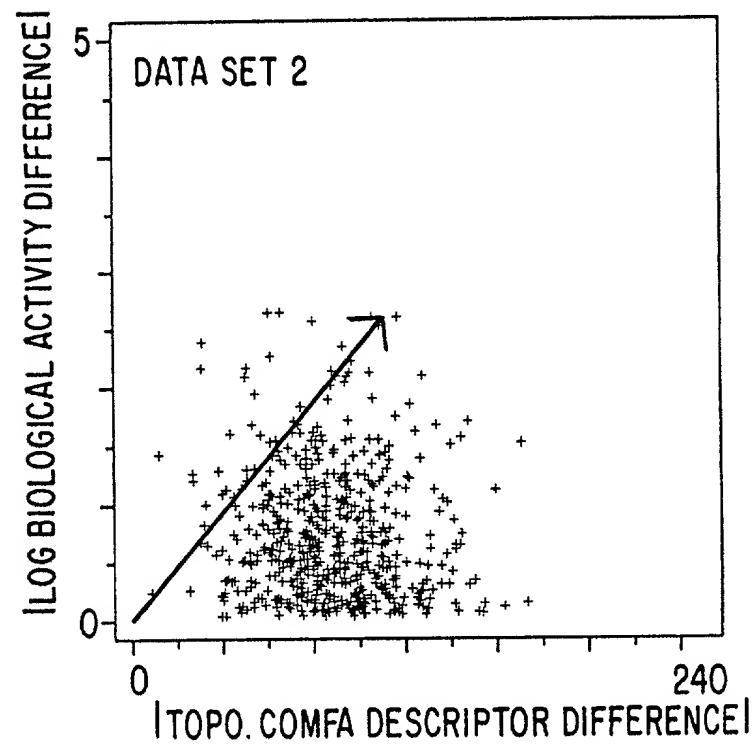


FIG.7(b)

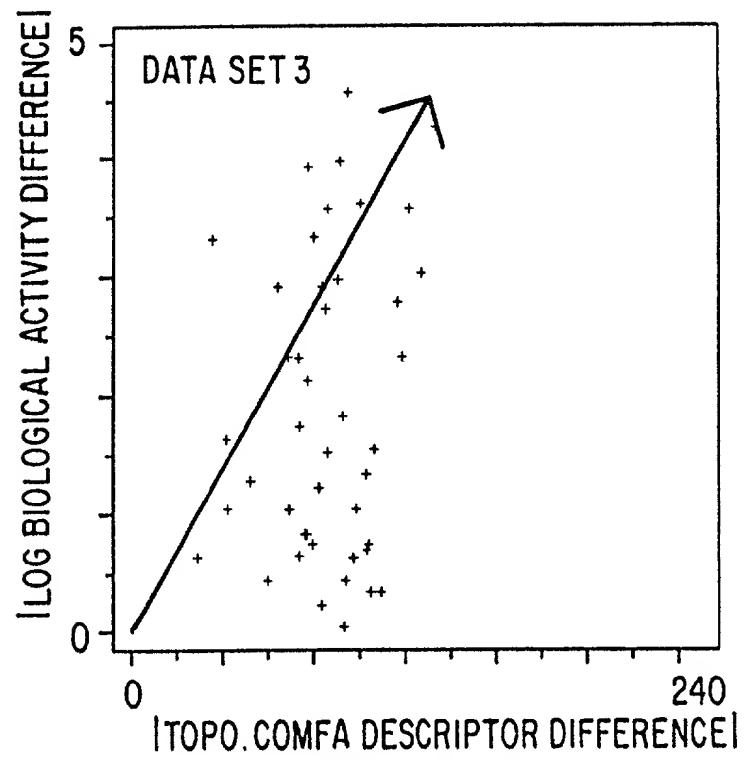


FIG.7(c)

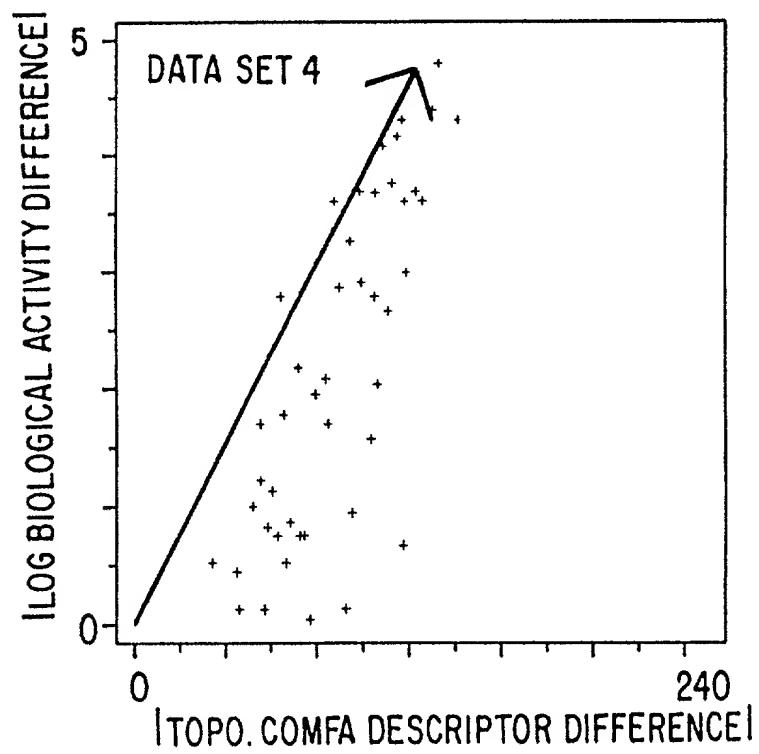


FIG.7(d)

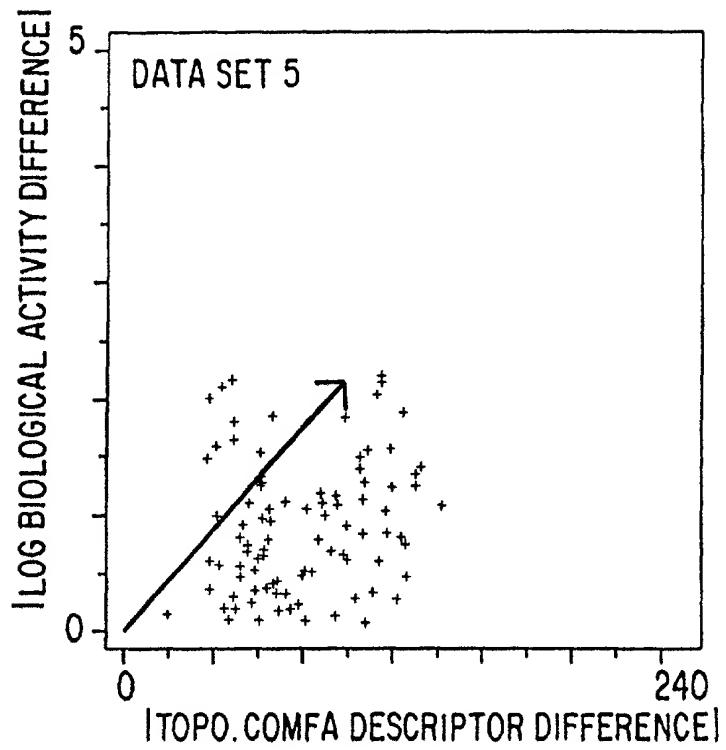


FIG.7(e)

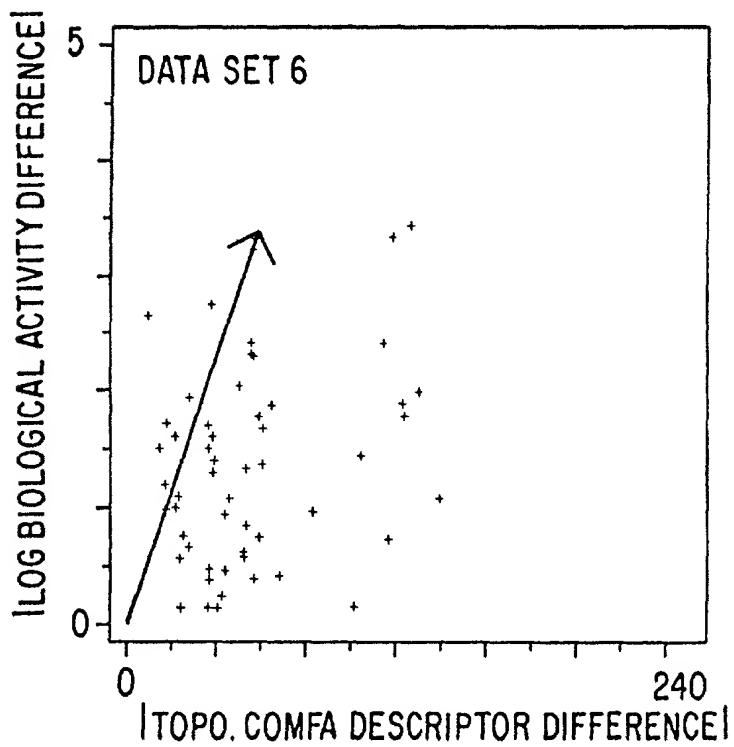


FIG.7(f)

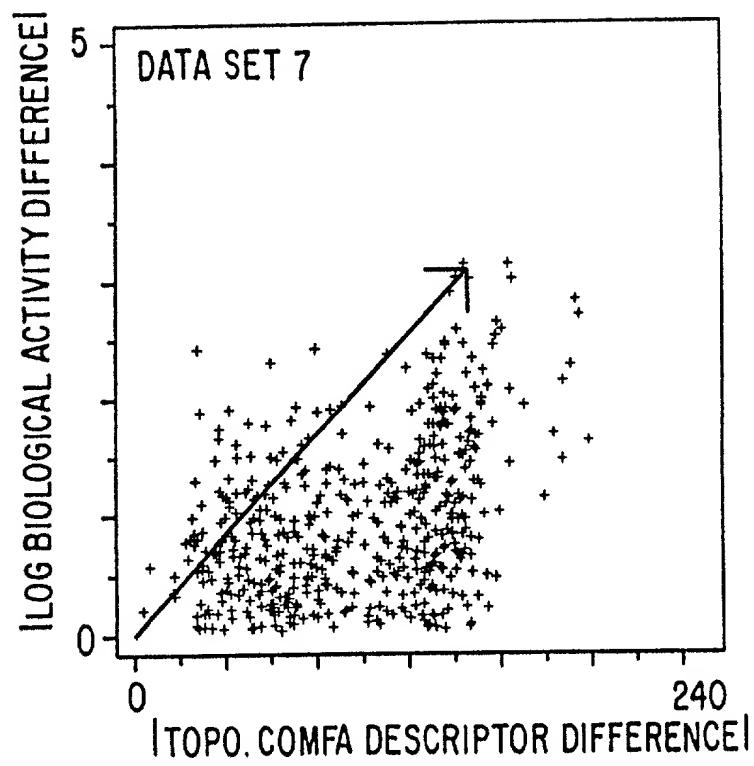


FIG.7(g)

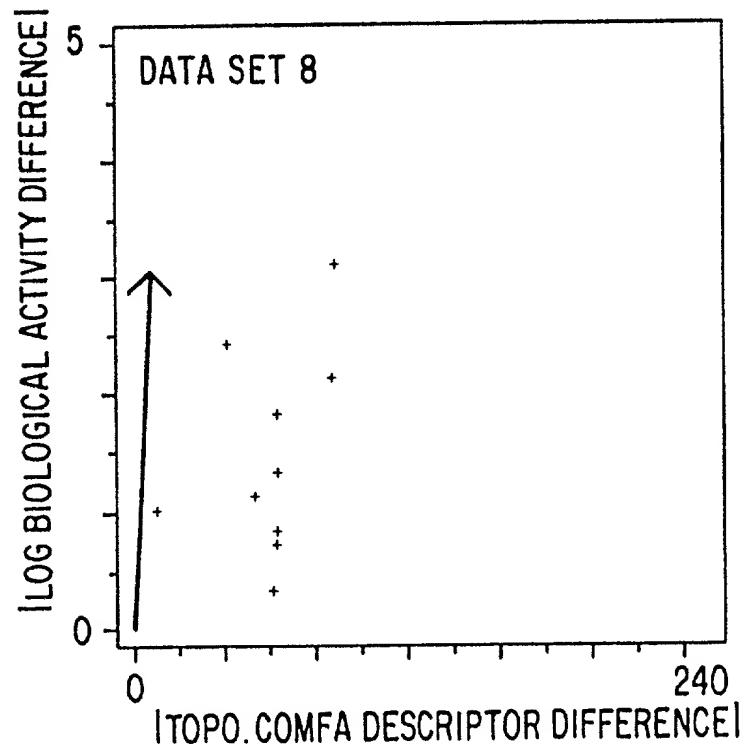


FIG.7(h)

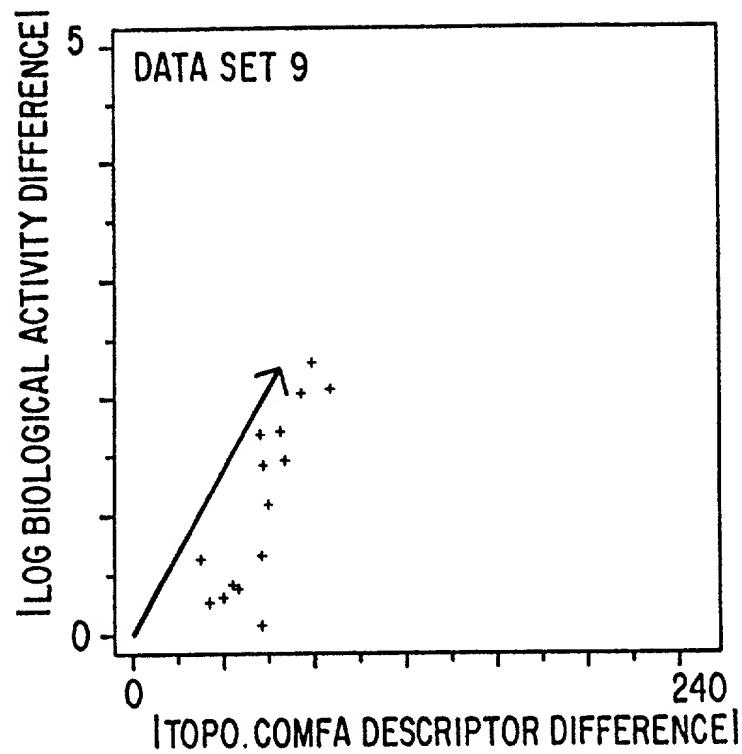


FIG.7(i)

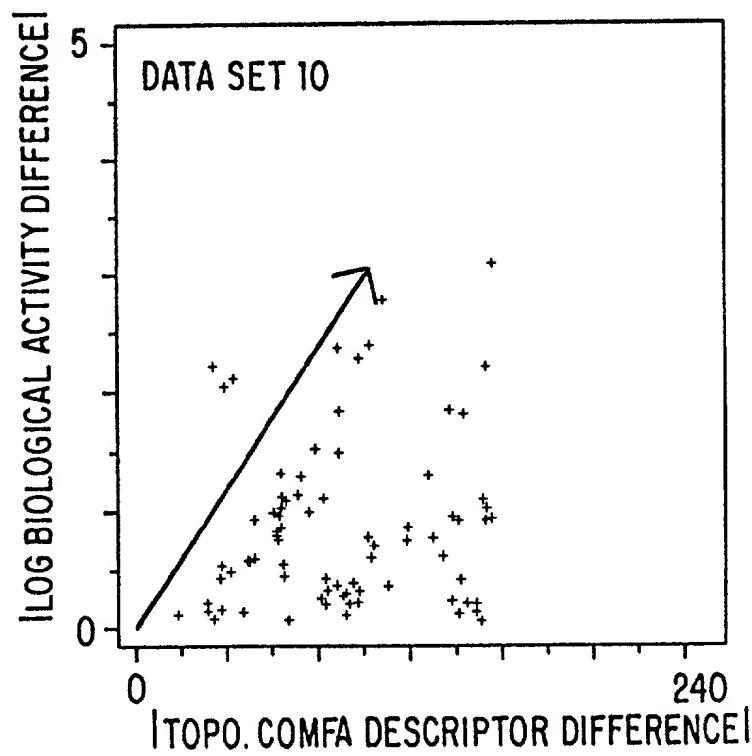


FIG.7(j)

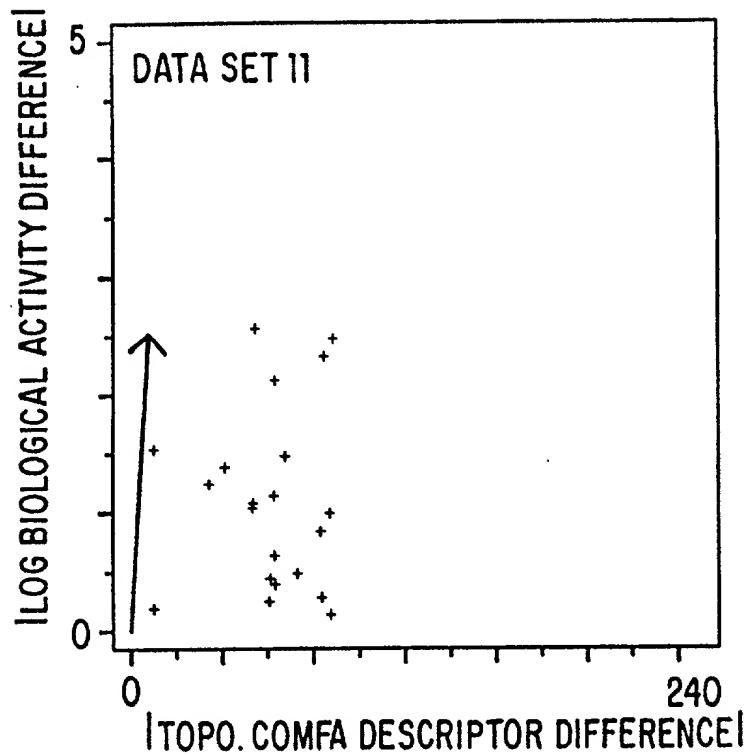


FIG.7(k)

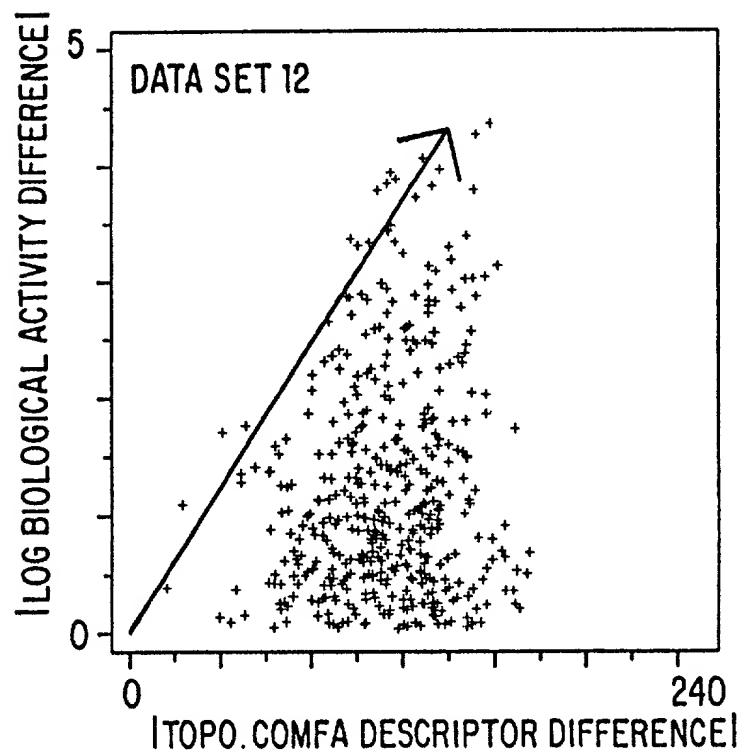


FIG.7(l)

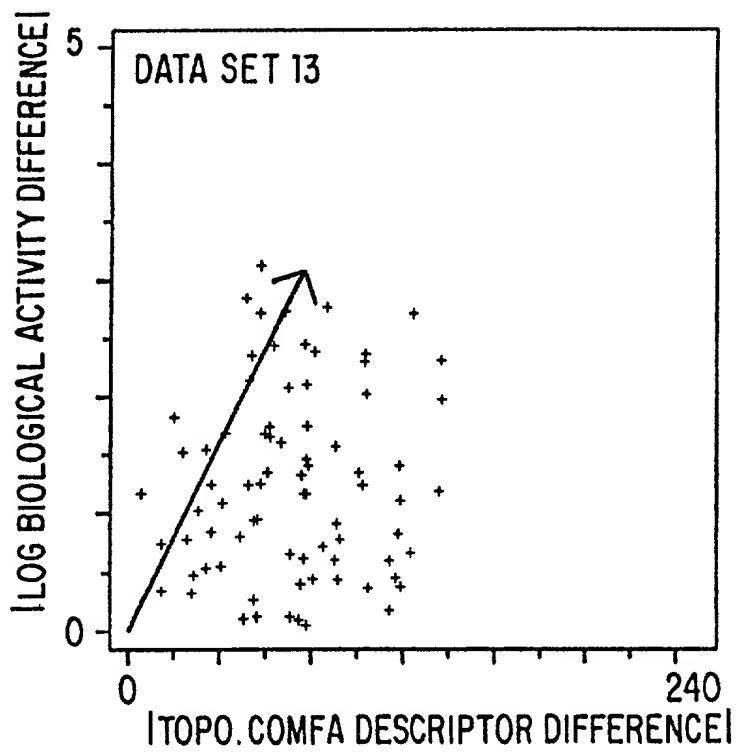


FIG.7(m)

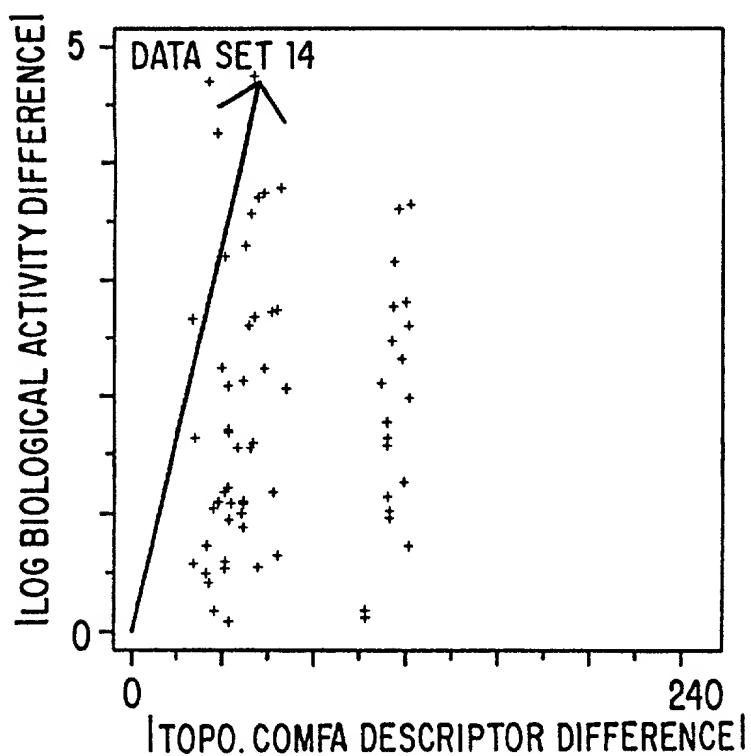


FIG.7(n)

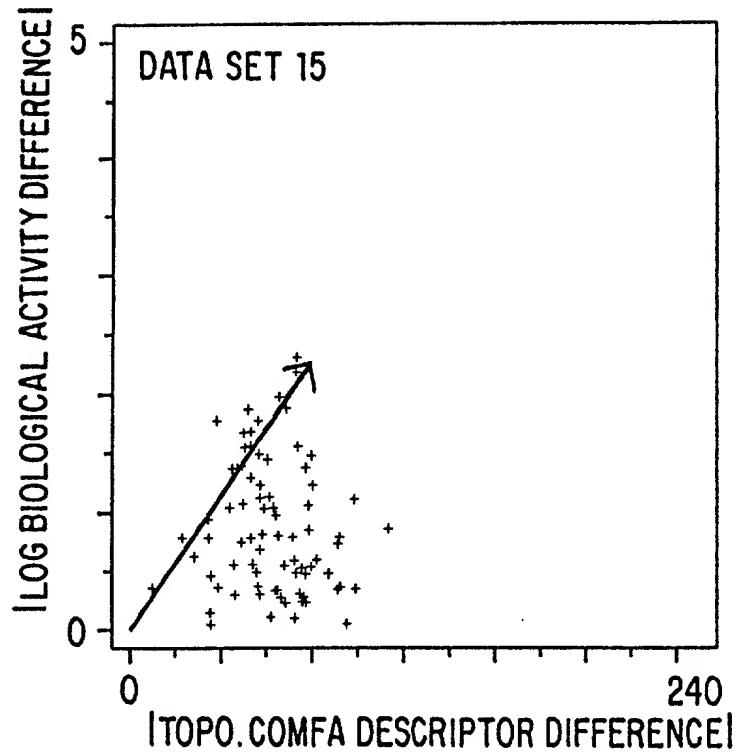


FIG.7(o)

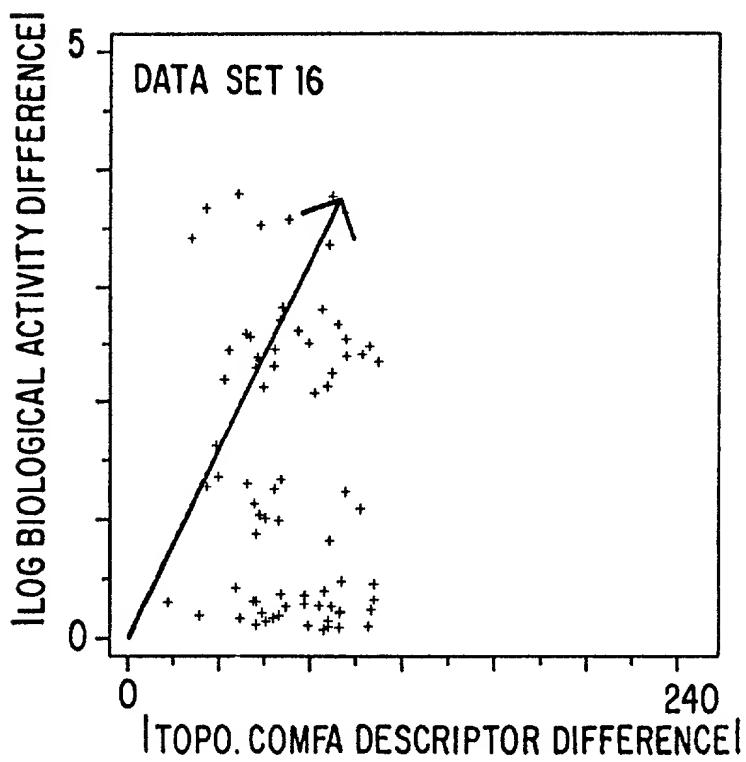


FIG.7(p)

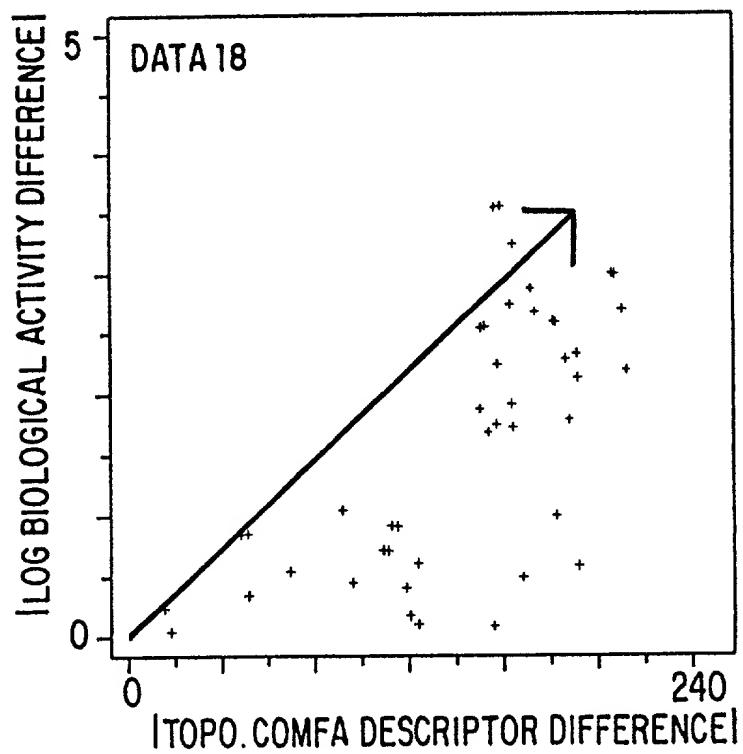
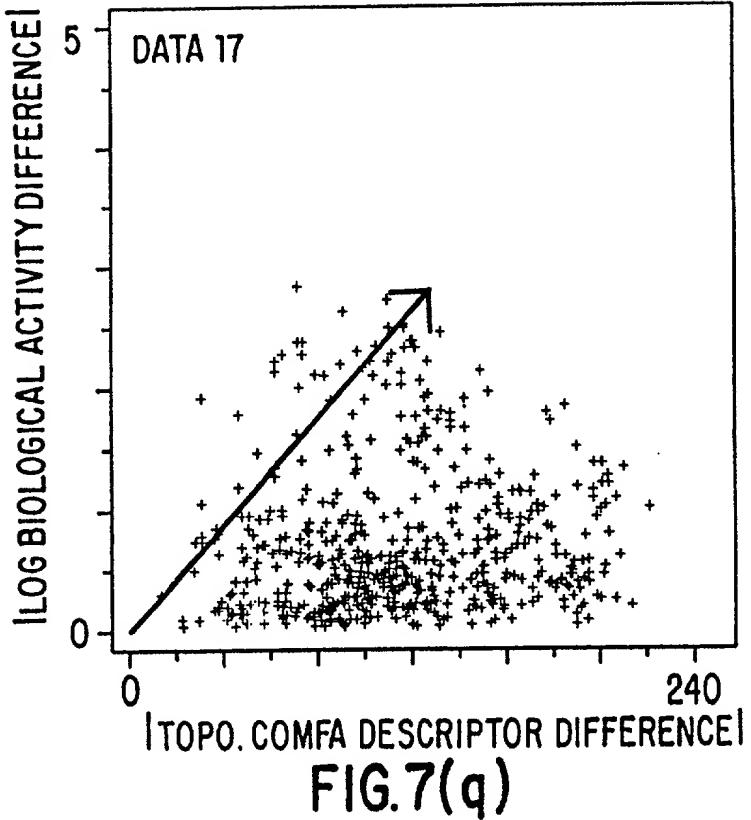


FIG. 7(r)

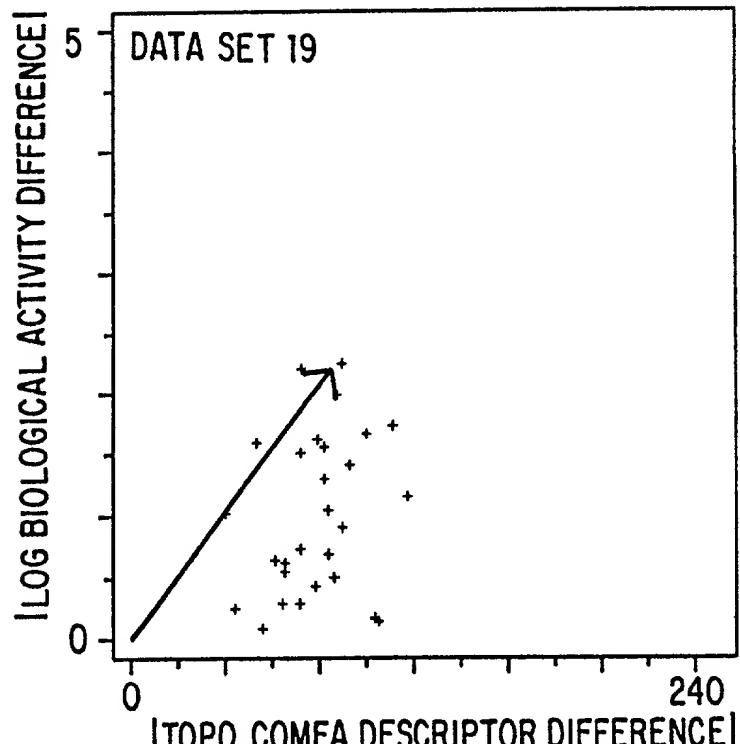


FIG. 7(s)

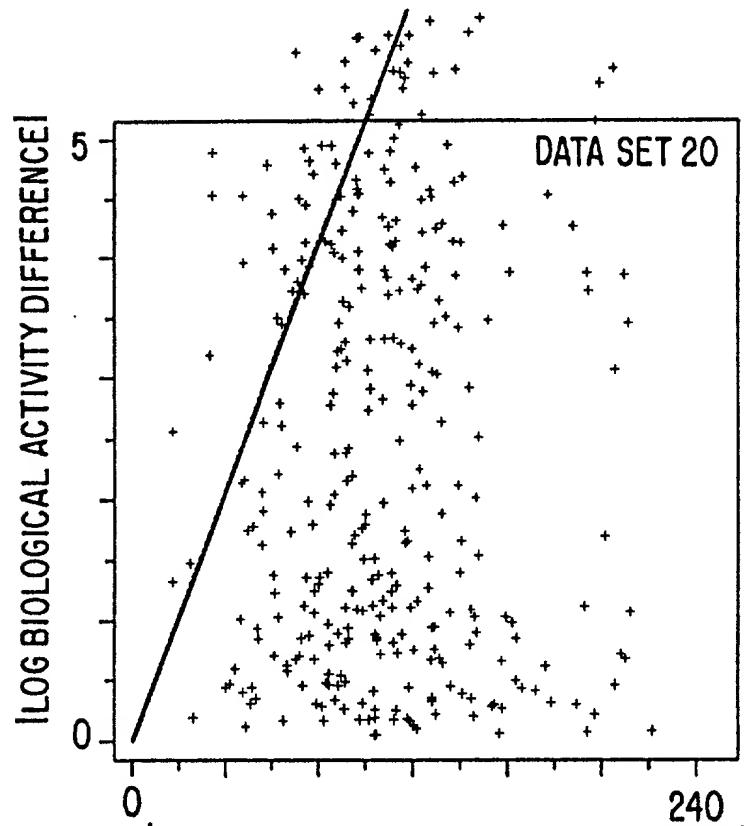


FIG. 7(t)

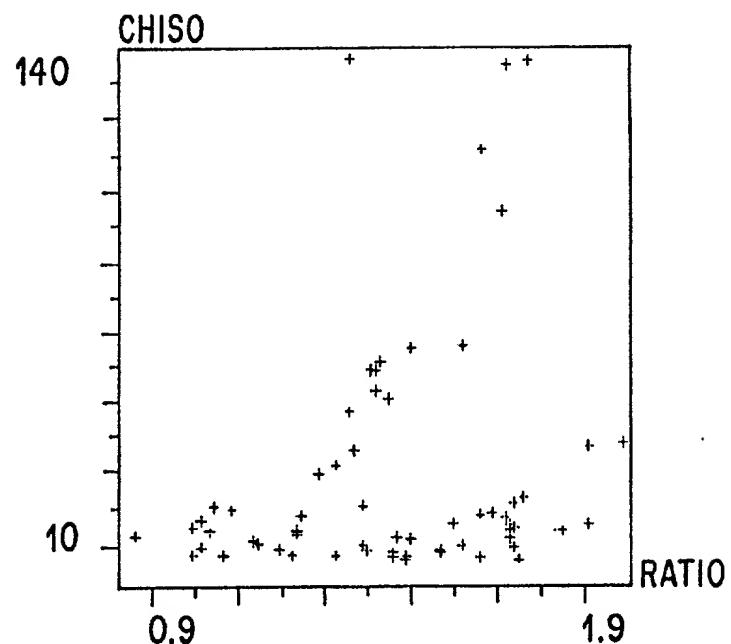


FIG. 8(a)

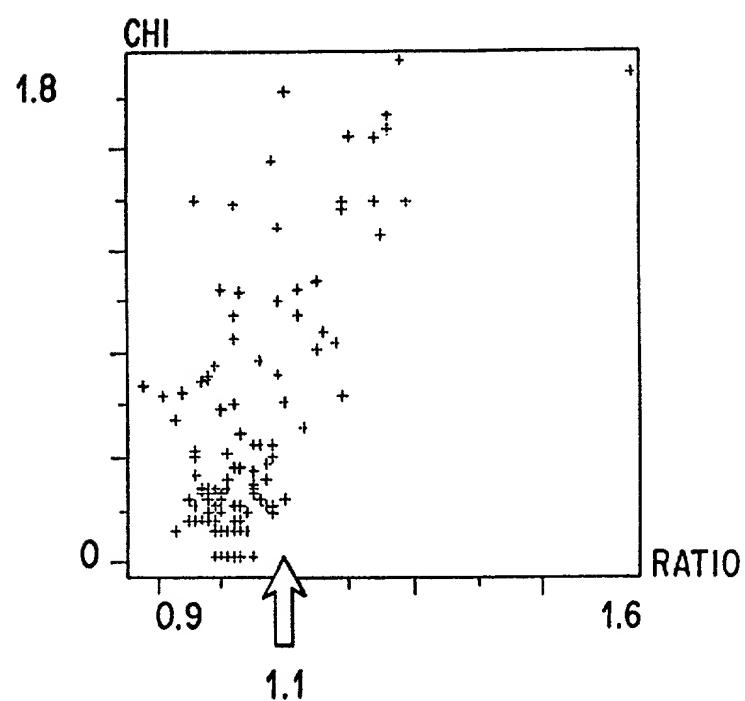


FIG. 8(b)

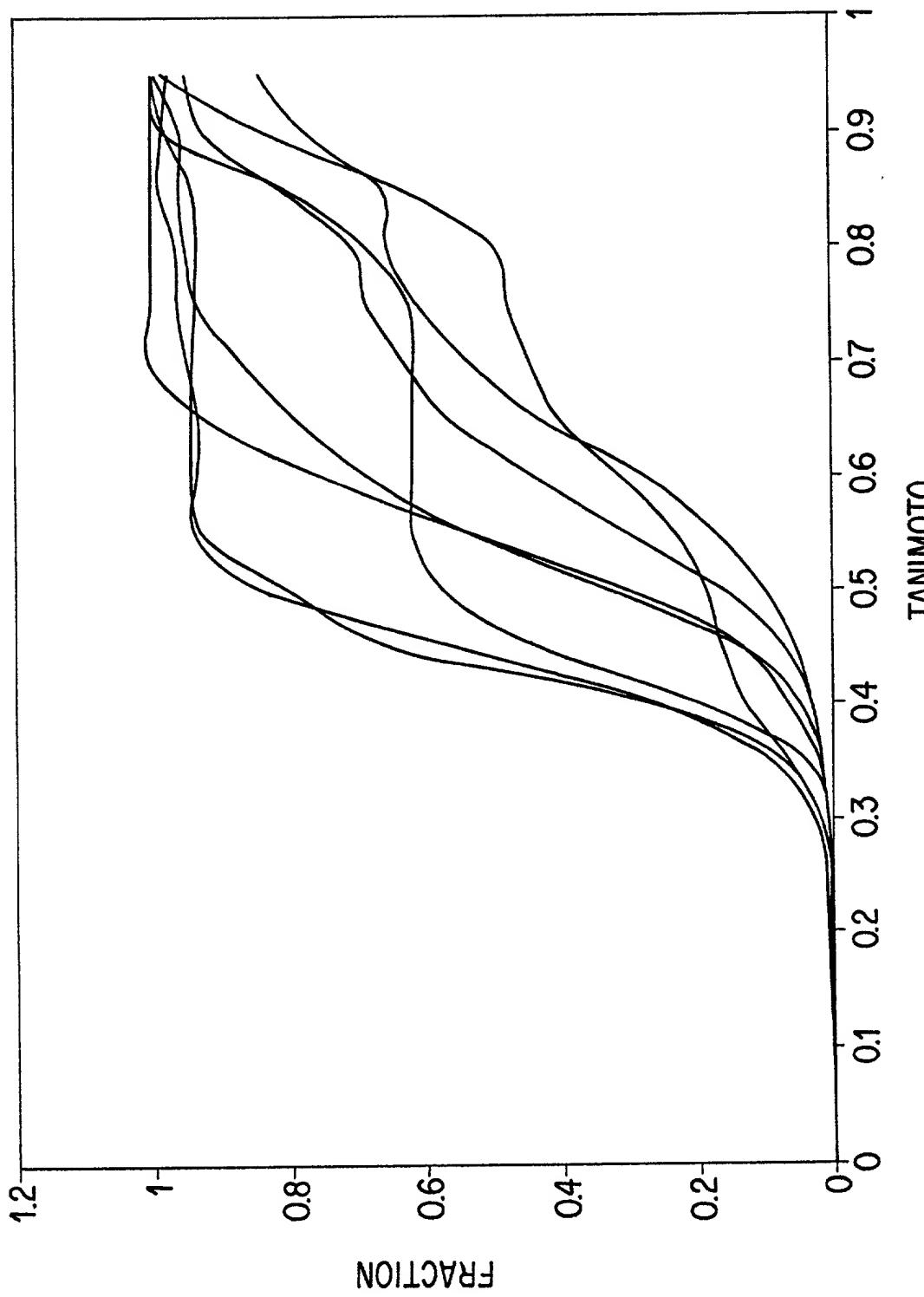


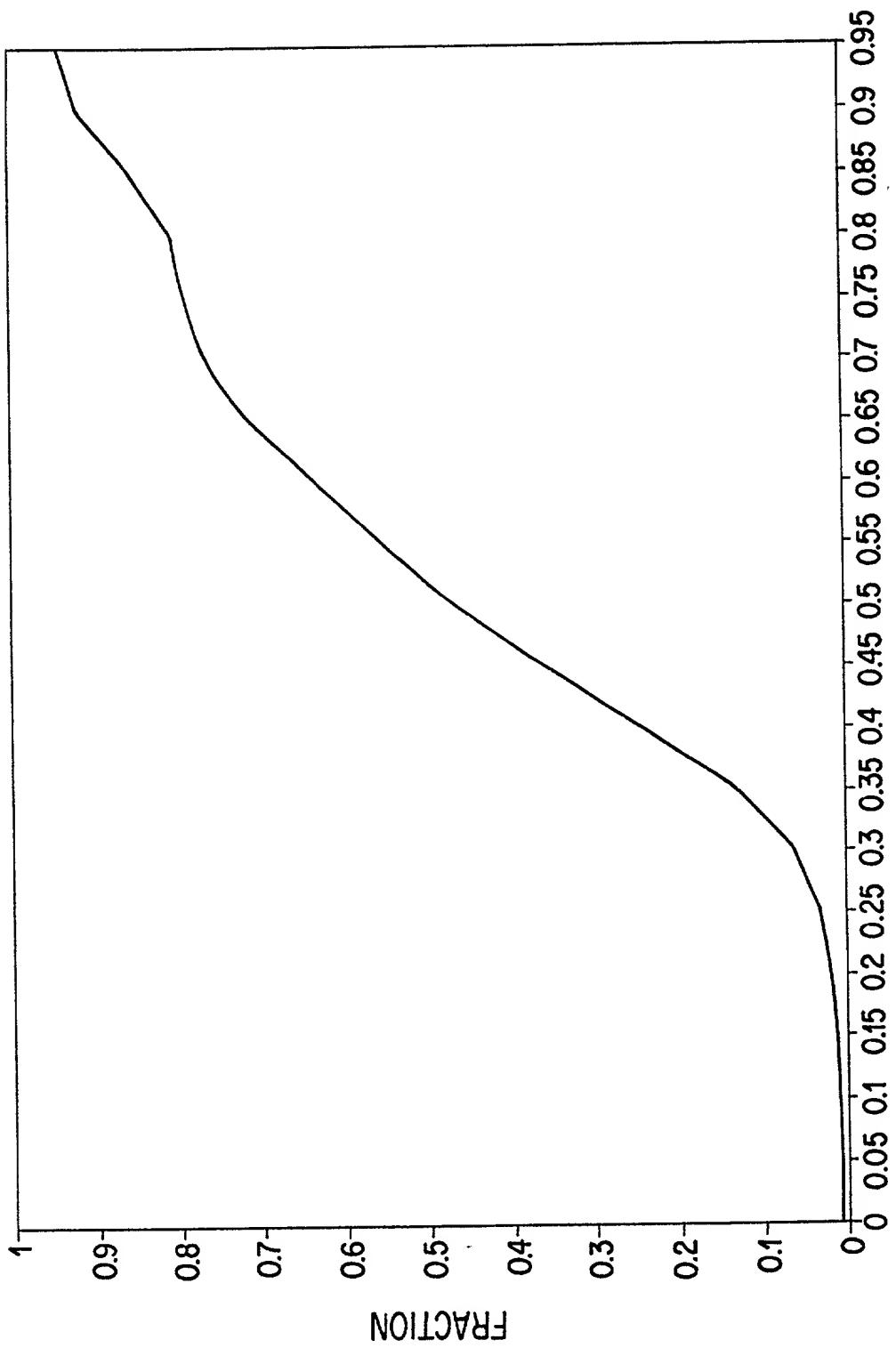
FIG. 9(a)

FIG. 9(b)



FIG. 9(c)

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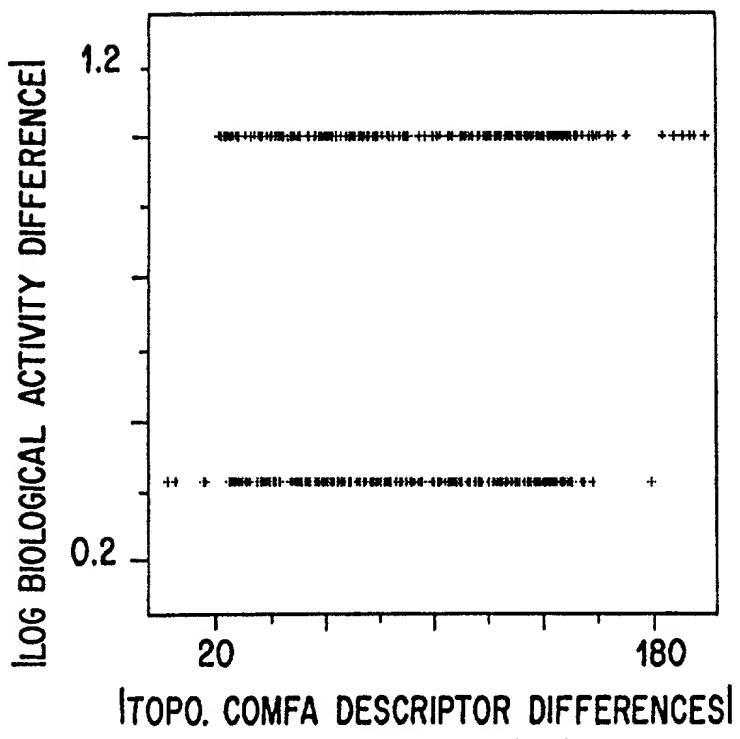


FIG.10(a)

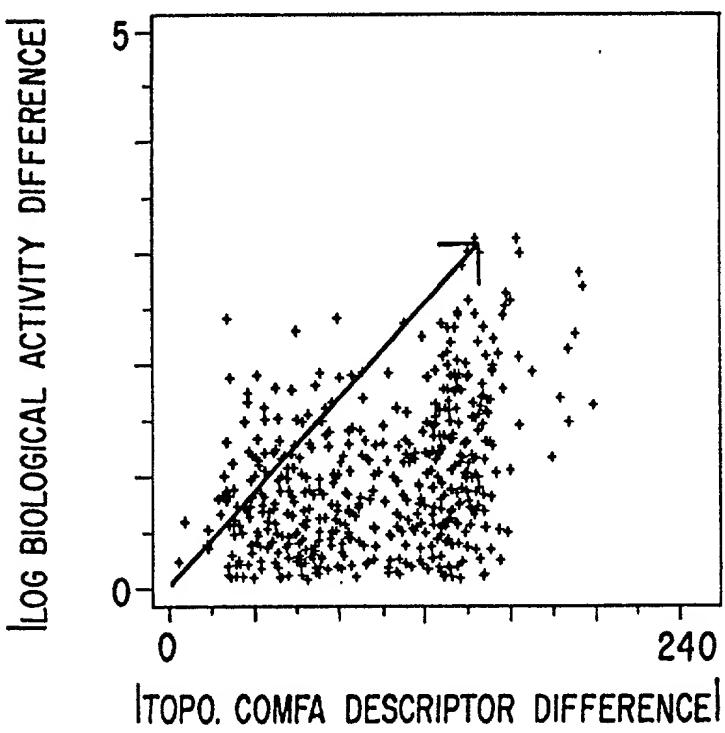


FIG.10(b)

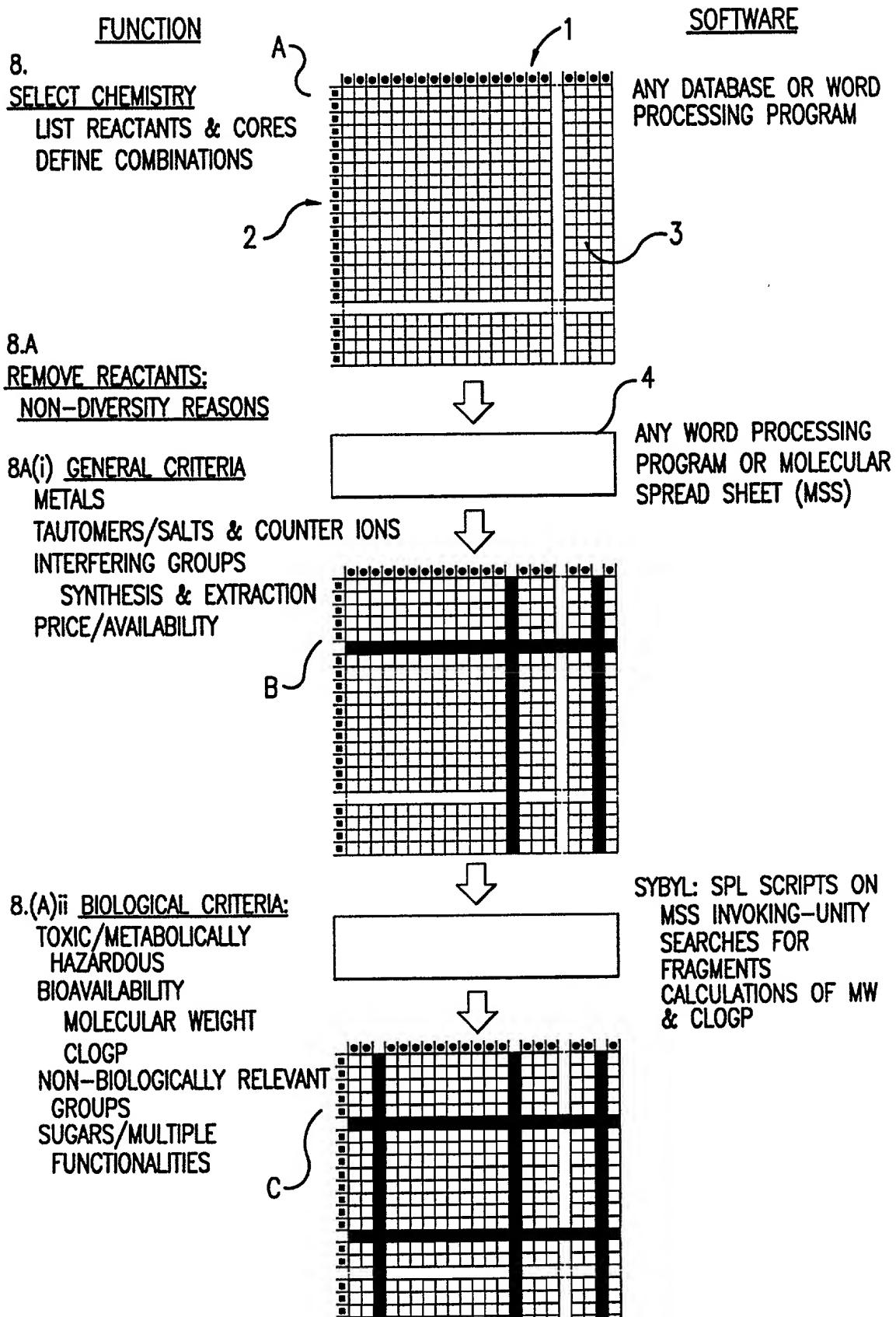


FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION

TOPOMERIC CONFORMER

ALIGNMENT

CoMFA FIELD GENERATION:

HYDROGEN BOND FIELD

GENERATION

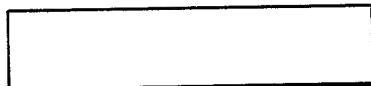
ROTATABLE BOND FIELD

ATTENUATION

CALCULATE FIELD
DIFFERENCES

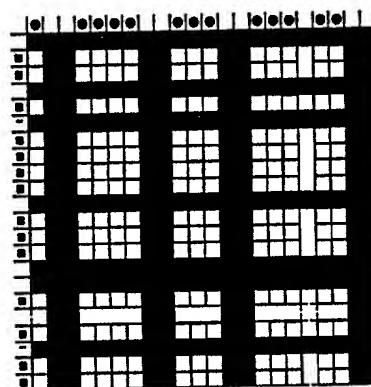
CLUSTER

REACTANT SELECTION FROM
EACH CLUSTER



SYBYL: SELECTOR &
CONCORD 3.2.1
SPECIALIZED SOFTWARE:
APPENDIX "A"
(SYBYL: CoMFA
STERIC & MSS)

SYBYL: HIERCHICAL
CLUSTER - MSS
SYLBL: MSS

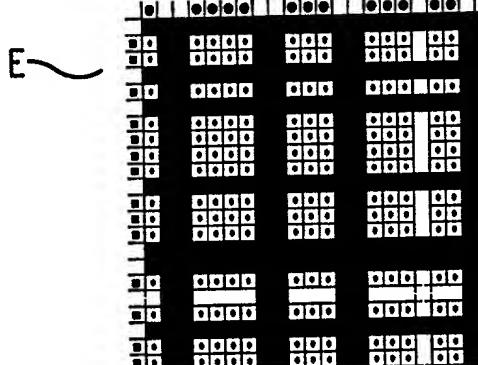


8C

COMBINE REACTANTS TO BUILD PRODUCTS



SYBYL: LEGION MSS



8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS



SYBYL: SPL SCRIPTS
ON MSS

GENERAL CRITERIA:

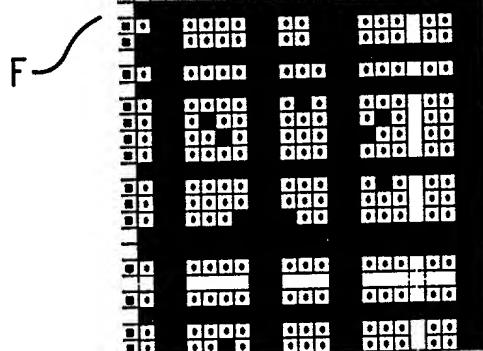


FIG.11(b)

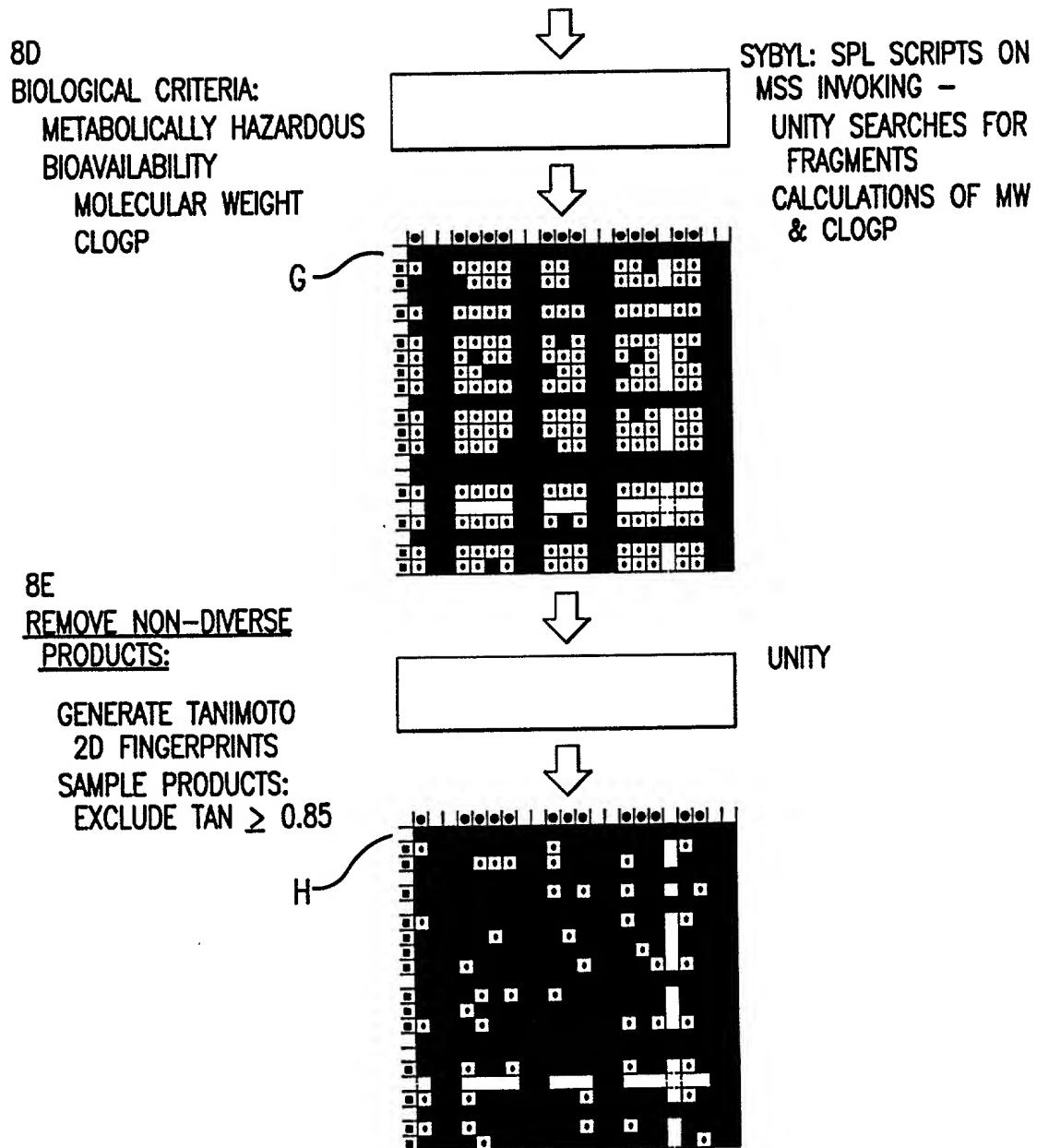


FIG.11(c)

FIG. 12

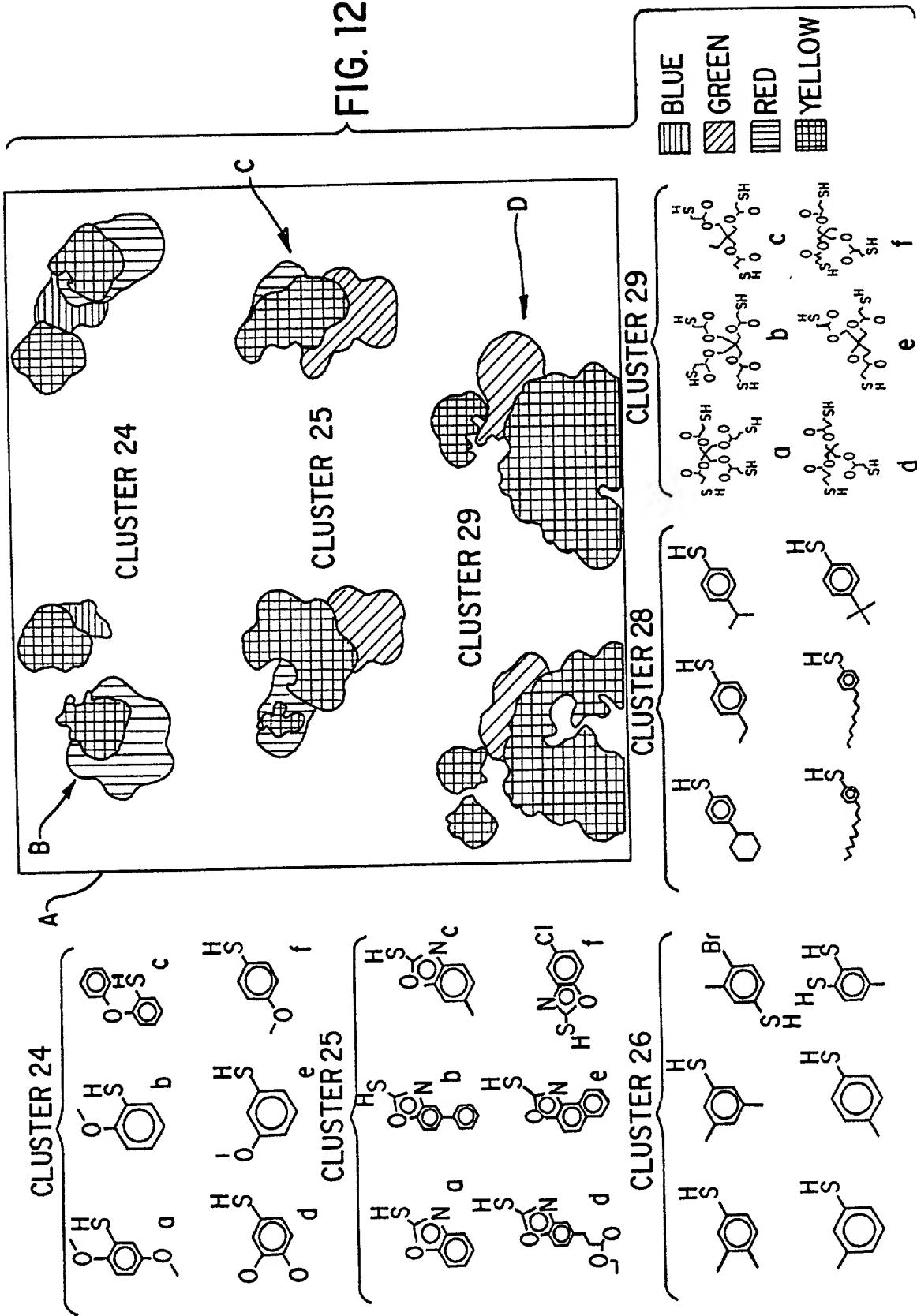


FIG. 13

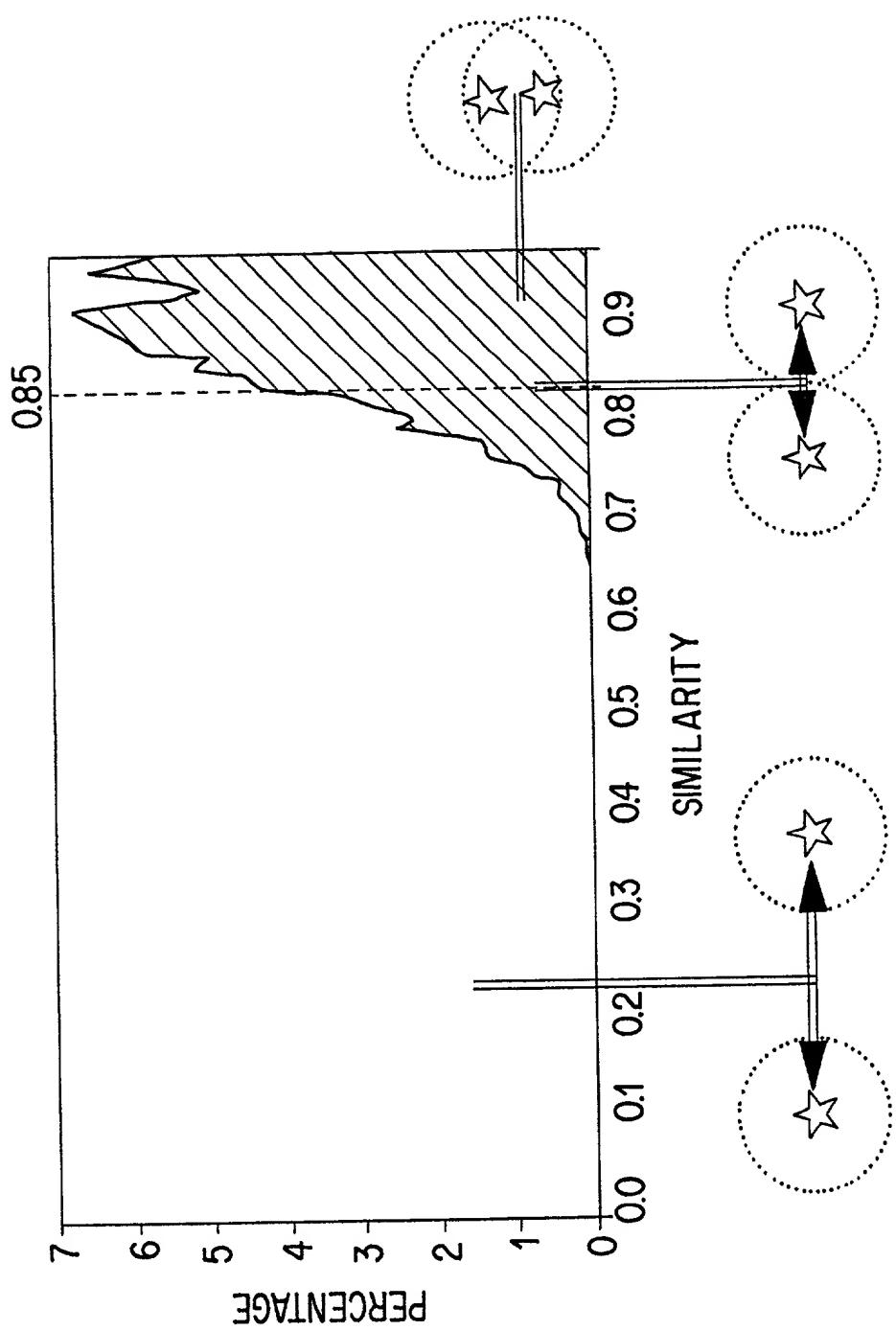
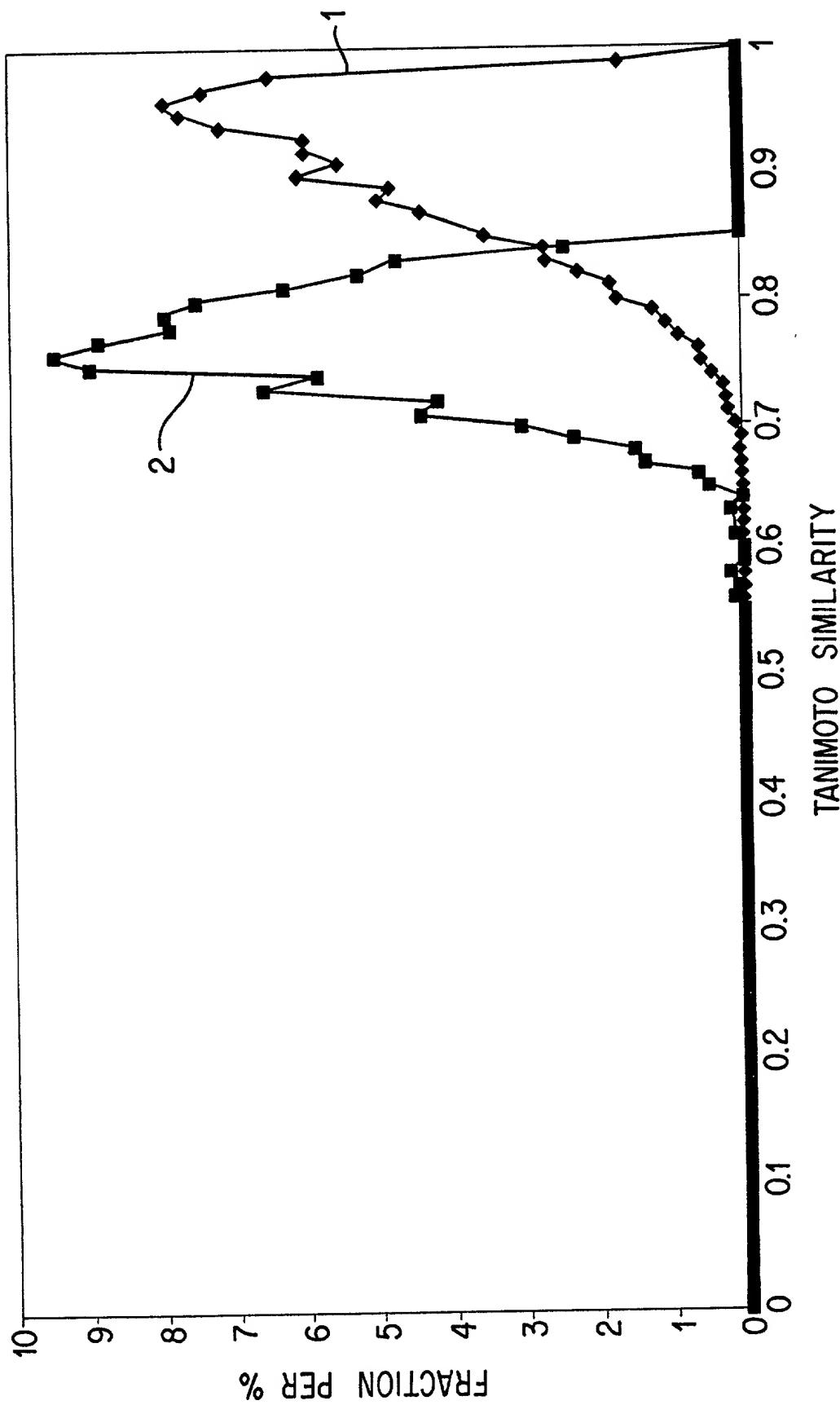


FIG. 14



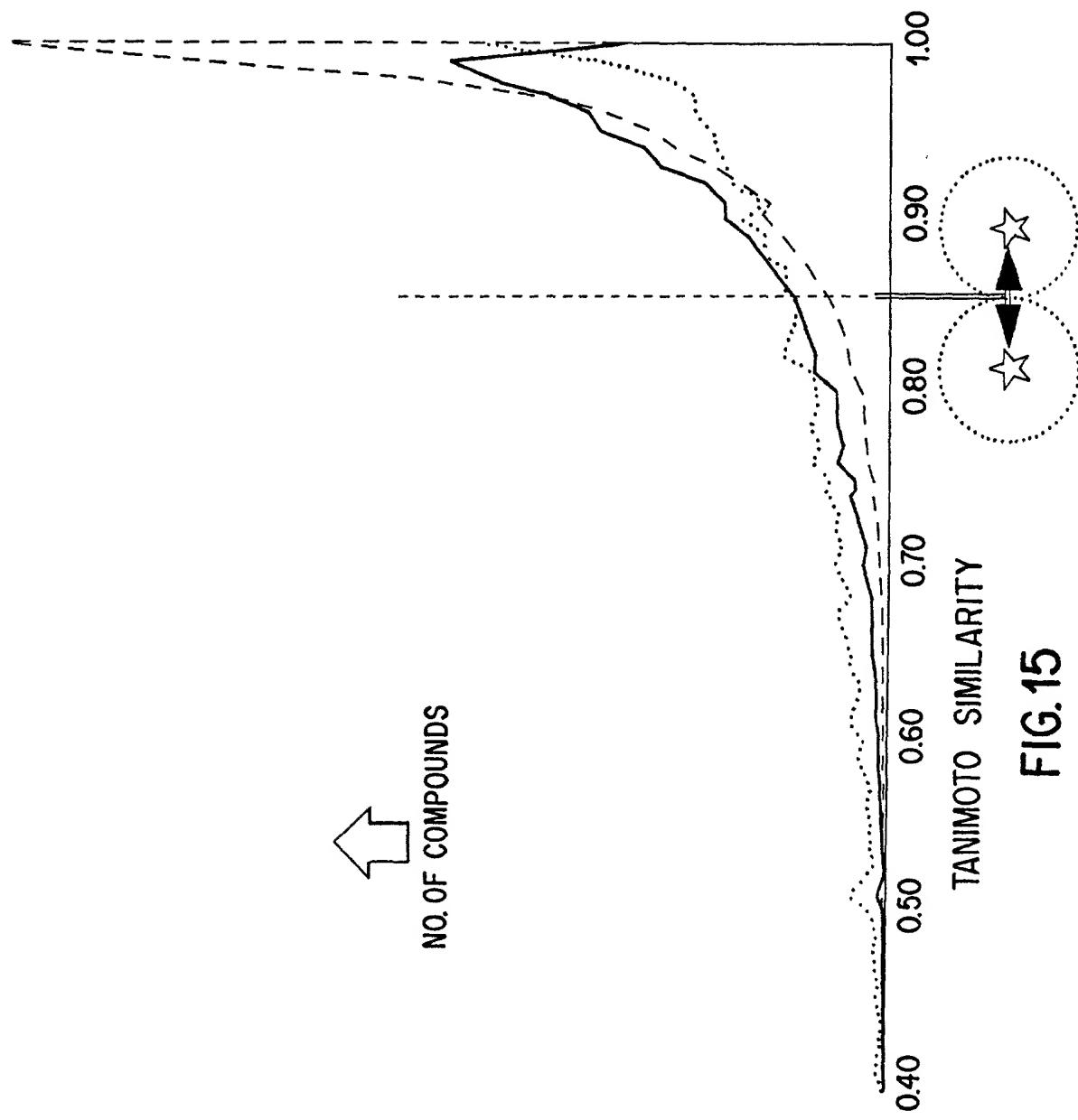


FIG. 15